Three Vignettes of the Equation of State and Transport in Dense Plasmas*

RIKEN-Brookhaven Workshop on Strongly Coupled Plasmas: Electromagnetic, Nuclear, and Atomic

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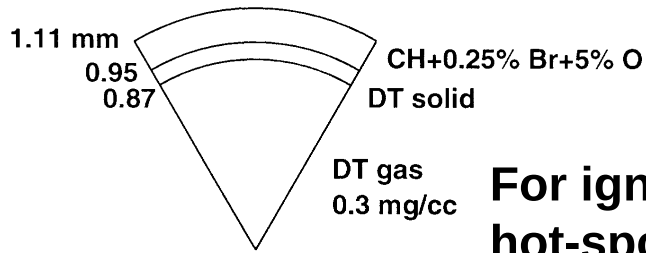
High Energy Density (Plasma) Physics: A Fascinating Interplay Between Applications and the Need to Understand Basic Physical Processes

- **In this talk I will present three experimental vignettes illuminating the measurement, computation, and understanding of basic phenomena**

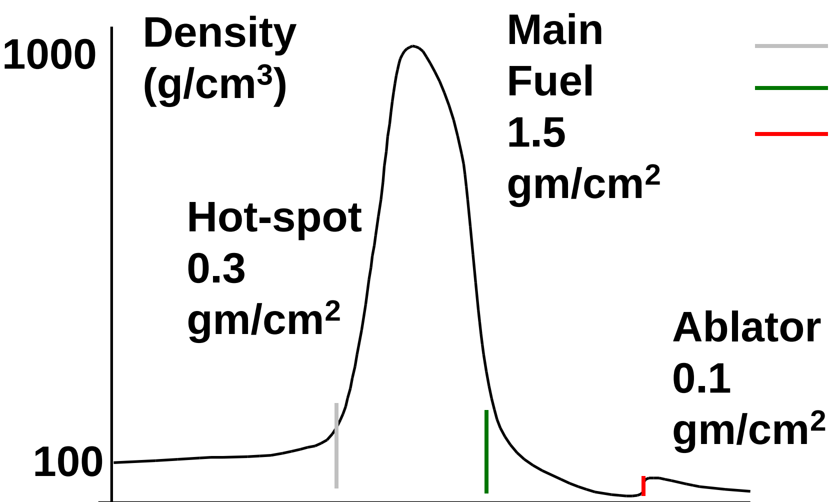
Application or Experiment	**Physics and Computational Topic**
1a) Inertial Fusion: convergent shock hot spot; fast ignition via short pulse laser **1b) K_α Source Generation as a diagnostic for short pulse generated fast electrons or x-ray source**	**Equation of State, dE/dx, and atomic excitation for nuclei and fast electrons**
2) Short pulse laser/matter interaction, pulsed power exploding wire dynamics	**$\varepsilon(\omega)$ and $\sigma(\omega)$ for reflectivity and local heating – interplay with the equation of state and 'continuum lowering.'**
3) Laser-plasma X-Ray Conversion, Dynamics of non-Planckian radiation – matter interaction, astrophysics (type 1a output)	**Local Thermal Equilibrium (LTE) and non-Local Thermal Equilibrium Radiation Transport (NLTE)**

'Hot Spot' Haan Ignition Target Design Relies on EOS and Alpha Particle Stopping in Compressed, Shocked Capsule

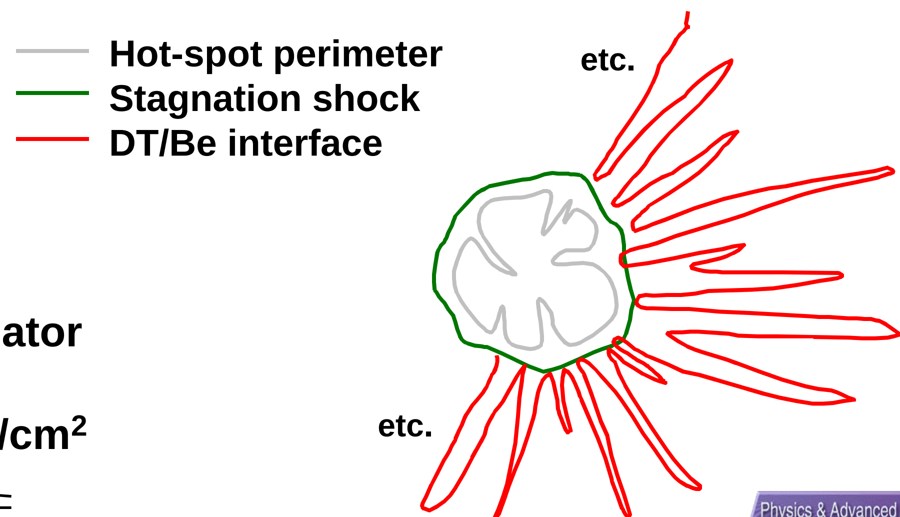


For ignition, need hot-spot with T_{ion} ~ 10 keV, ρR_{HS} ~ 0.3 g/cm^2

1D picture



2D or 3D picture



Alpha Particle Ranges are Strongly Temperature Dependent and Importantly Depend on Both Ions and Electrons

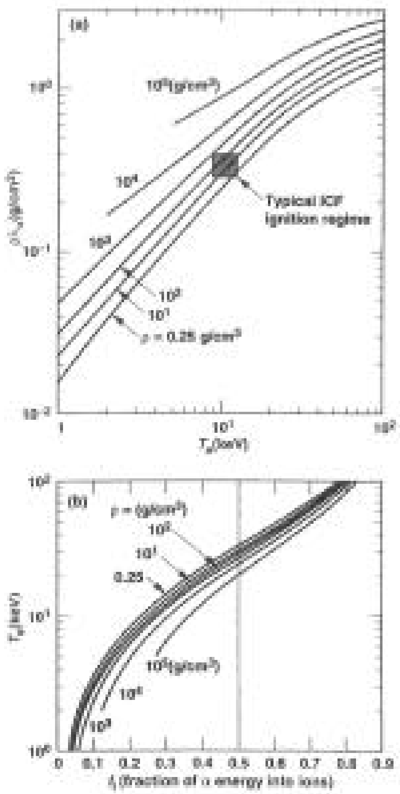


FIGURE 1.4. Efficient alpha capture requires $\rho r \sim 0.3$ g/cm^2. (a) Alpha-particle range $\rho\lambda_\alpha$ vs T_e; (b) alpha-energy absorption.

$$\frac{dU}{dx} = -26.9\frac{\rho}{\rho_0}\frac{U^{1/2}}{T_e^{1/2}}\{1+1.68\ln[T_e\left(\frac{\rho}{\rho_0}\right)^{1/2}\}-.055\frac{\rho}{\rho_0}\frac{1}{U}\{1+.075\ln[T_e^{1/2}\left(\frac{\rho}{\rho_0}\right)^{1/2}U^{1/2}\}$$

1st Term is due to electrons, 2nd is due to ions. Temperature Dependence Due to Frame effect. (Fraley et. al. Physics of Fluids 1974. ρ_0 is solid DT density (.25 gr/cc).

J. Lindl, Inertial Confinement Fusion, Springer, 1998.

dE/dx in a Plasma via Dimensional Regularization (L. Brown, PRD 2000)

- dE/dx depends both on long distance, collective joule heating effects and hard short distance Coulomb Scattering Effects. These are separately divergent in 3 dimensions.
- Brown's idea is to sum the analytic continuations of the $\nu>3$ scattering and the $\nu<3$ joule heating to get a finite result including subleading terms.
- Example shown has $v_p \gg v_{thermal}$. One can compute for arbitrary T_e using general form for $1/\varepsilon(\omega,\kappa)$.

$$\frac{dE_<}{dt} = e_p^2 \int \frac{d^\nu k}{(2\pi)^\nu} \frac{1}{k^2} \mathrm{Im}\left\{ \frac{-k\ v_p}{\varepsilon(k, k\ v_p)} \right\}$$

$$\frac{dE_>}{dx} = \frac{n_e}{2m_e} \int d\sigma q^2 \to \frac{e_p^2 \omega_e^2}{4\pi v_p^2} \left(\frac{4\pi m^2 v_p^2}{h^2} \right)^{\frac{\nu-3}{2}} \left\{ \frac{1}{\nu-3} + \frac{\gamma}{2} \right\}$$

$$\frac{dE}{dx} = \frac{e_p^2 \omega_e^2}{4\pi v_p^2} \ln\left(\frac{4\pi m v_p^2}{h \omega_e} \right)$$

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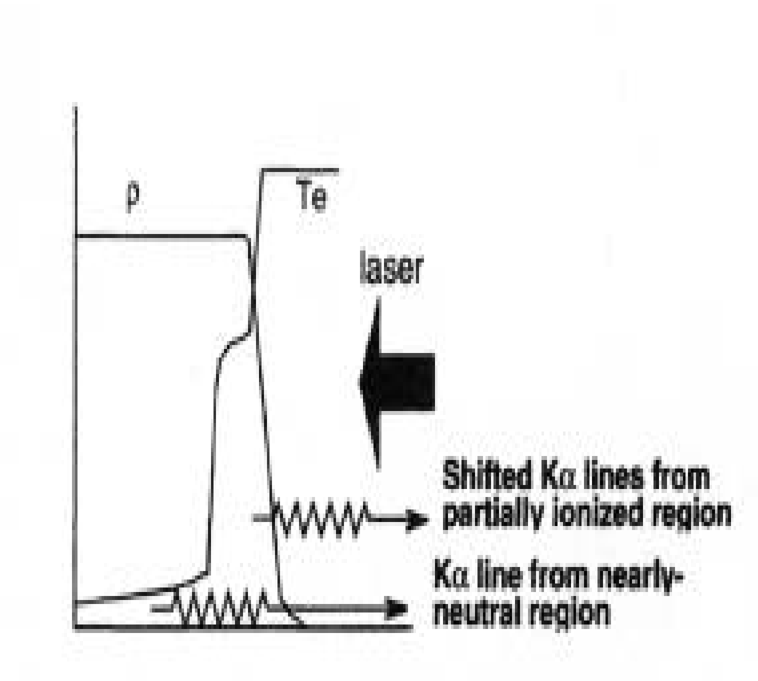
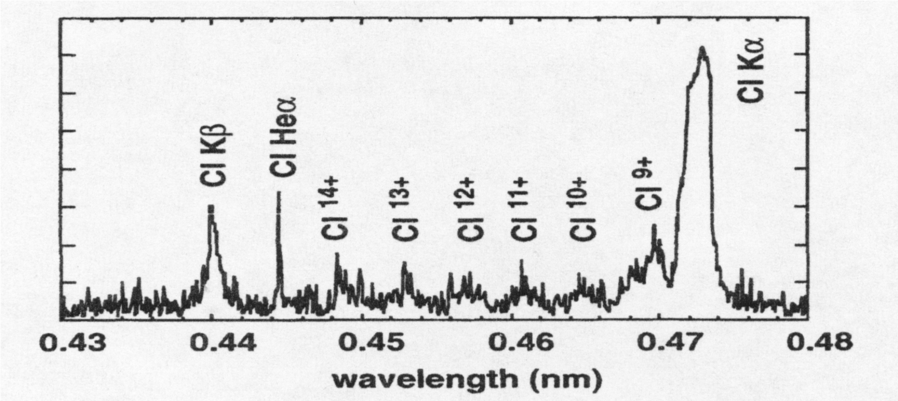
Atomic Physics Considerations for Kα Emission

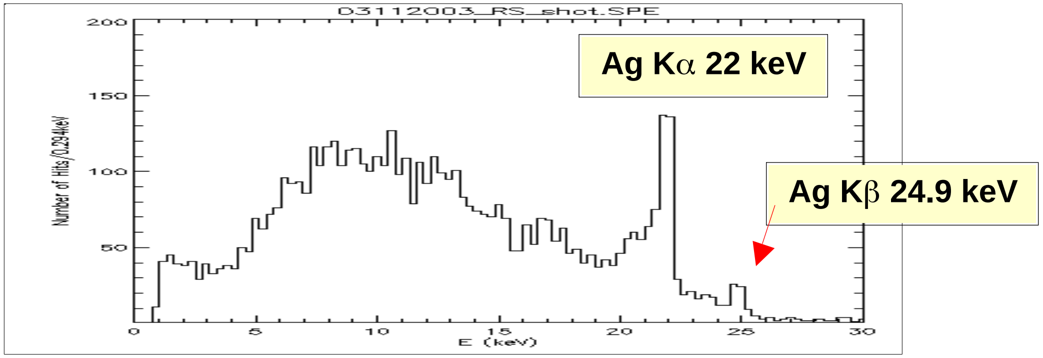


Kα emission depends on e- transport and atomic processes over a wide temperature range

Cl-CH 50 mJ 10^{17} W/cm^2 (Nichimura '02)



Ag 192 J Vulcan 2×10^{17} W/cm^2 (H-S Park '03)



Atomic Physics Enters Short Pulse Experiments both as Microscopic Quantities and in Integrative Modeling

- K_α experiments serve both a fast electron velocity distribution and dE/dx diagnostic and for the development of petawatt driven hard x-ray backlighters. Interpretation of experiments requires attention to atomic physics issues.
  - Detailed relativistic energy shifts and electron impact cross sections are required to get an accurate picture of the emission spectra and fluorescent yield.
  - The problem of the relaxation of a non-Maxwellian electron distribution in the presence of NLTE atomic physics is analogous to that of NLTE radiation transfer.
  - Radiation trapping?

Kα Energy Shifts are Calculated from the MCDF ‘No-Pair’ Relativistic Hamiltonian (M. Chen)

$$H_{\text{no-pair}} = \sum_{i=1}^{N} h_i + \Lambda_{++}(H_C + H_B)\Lambda_{++}$$

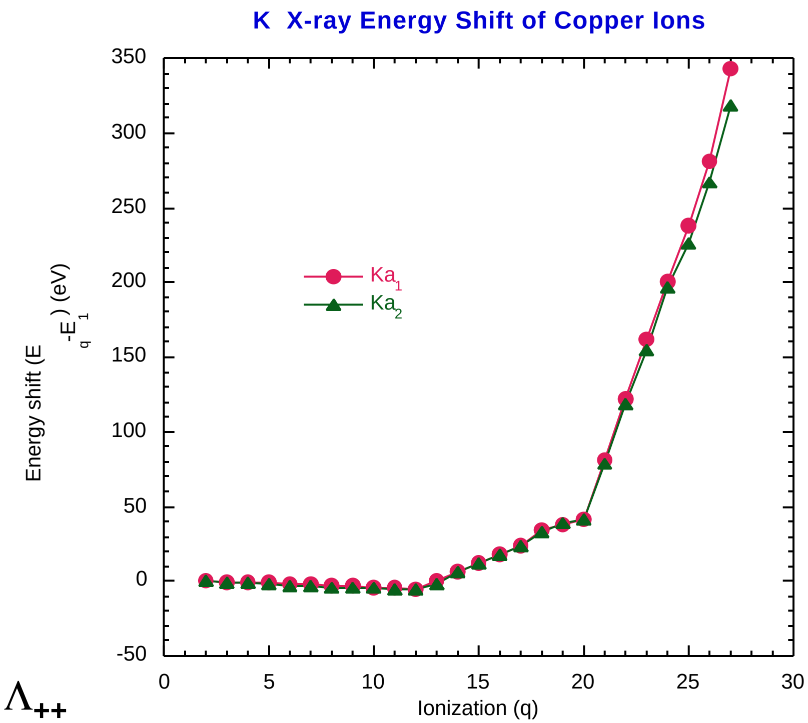
Atomic eigenstate function

$$\Psi(JM) = \sum_i c_i \phi_i(JM)$$

$$H\Psi = E\Psi$$

Variational MCDF equation

$$\sum_j (H_{ij} - \lambda\delta_{ij})c_j = 0$$



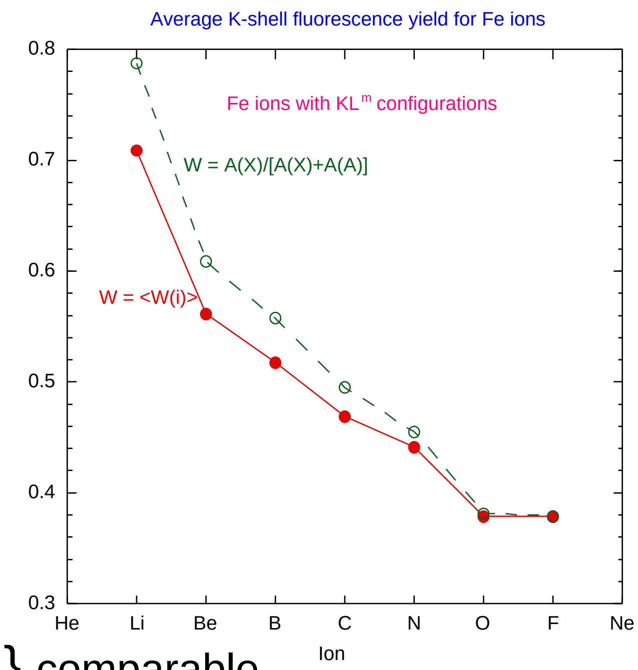
- **Positive-energy projection operators Λ_{++}**
- **Eigenenergy λ and eigenvector {ci} are obtained by diagonalizing the Hamiltonian matrix Hij**
- **Accuracy 1.5 eV out of a few keV - sufficient for shifted Kα emission of M-shell Cu ions (4eV).**

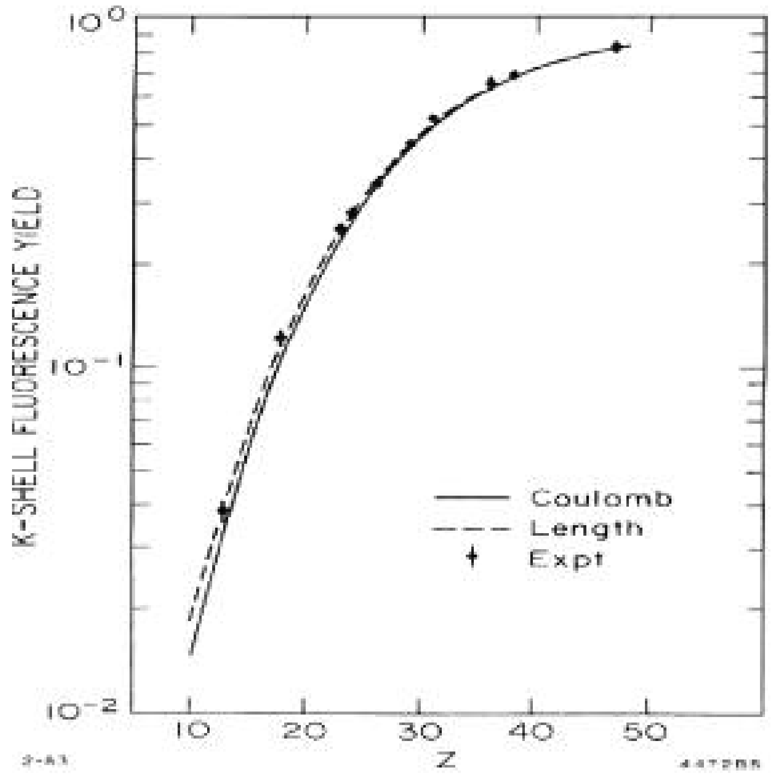
X-Ray fluorescence Yields Depend on Ionization and Must Correctly Include Selection Rules (M. Chen)

$$\overline{\omega} = \frac{\sum_{L,S}(2L+1)(2S+1)\omega(LS)}{\sum_{L,S}(2L+1)(2S+1)}$$

K-shell yield $\omega(K)$=0.46
E(Kα1)=8047.4 eV)
E(Kα2)=8027.3 eV
Natural line width
G(Kα1)=2.1 eV
G(Kα2)=2.5 eV
Lifetimes
--K- hole =4.3x10^{-16} s
--L_3- hole =1.2x10^{-15} s

Competing processes:
Radiative decay
Auger decay } comparable
Collisional processes - 3B, DX smaller





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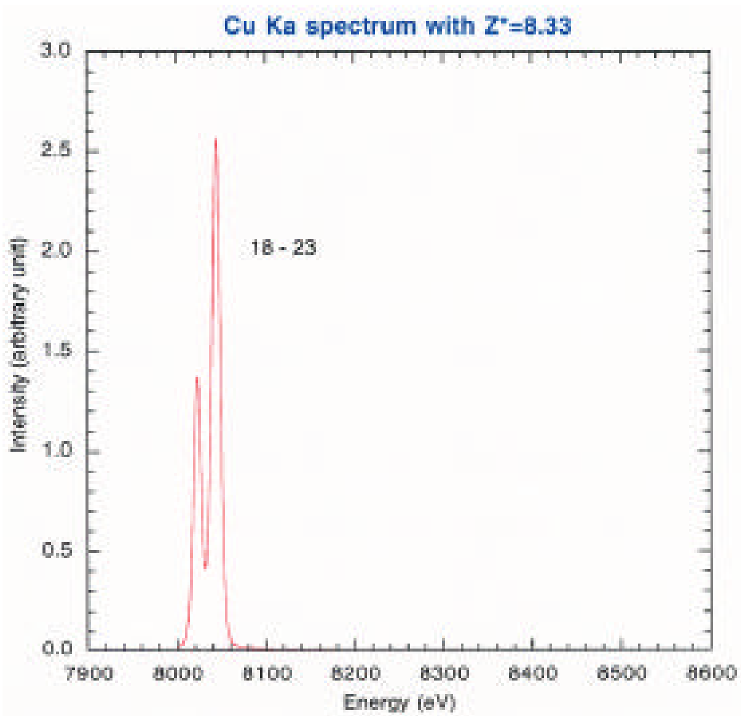
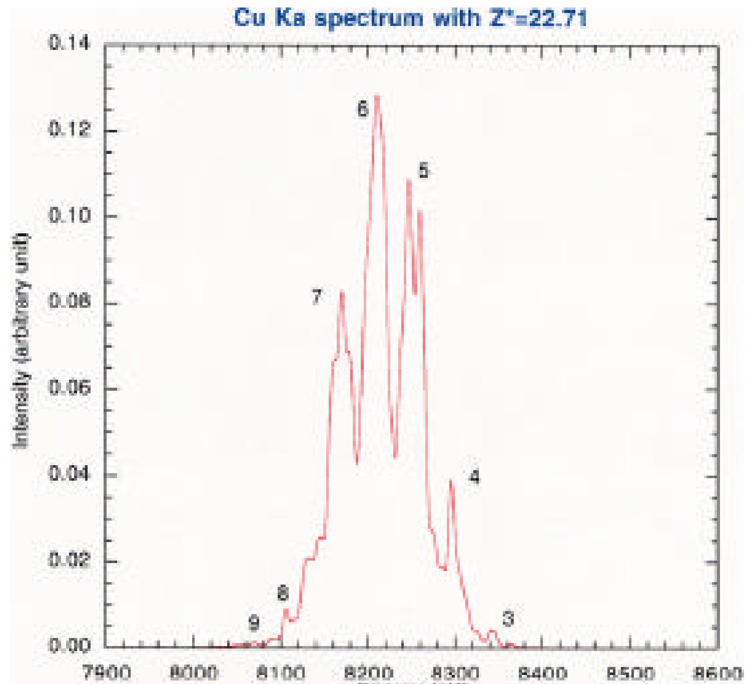
Synthetic K Shell Spectra Including Ionization Effects (Shifts and Branching Ratios) (M. Chen)

Calculations assume thermal ion distribution and use 8 eV instrumental width



2p spin-orbit splitting dominates in M-shell



Multiplet splitting dominates in L-shell

Measuring L-shell shifts (~40 eV per charge state) should be feasible

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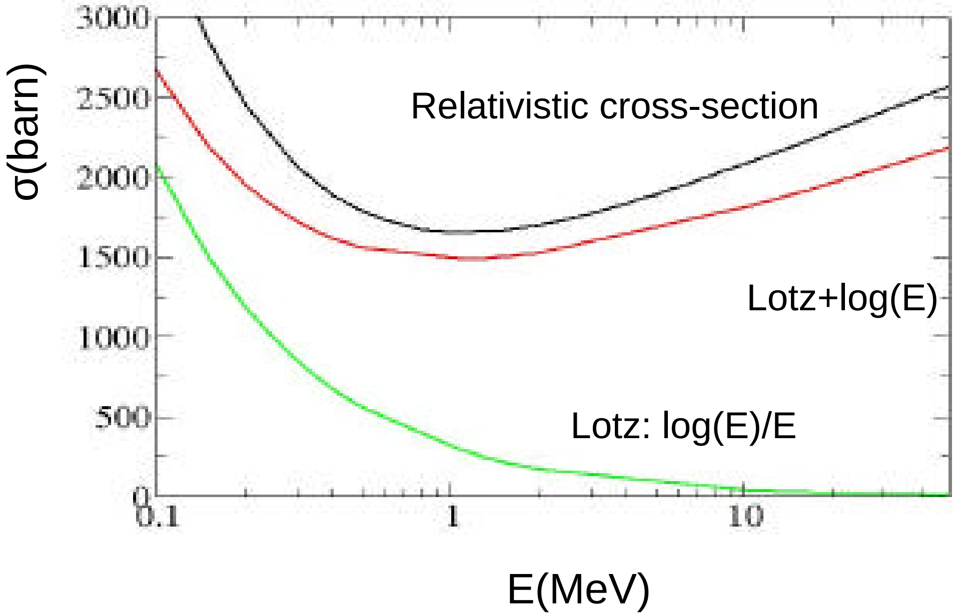
Relativistic Electron IonizationCross Sections Scale Asymptotically like the Møller Cross Section (1)

- **Non-relativistic approximations include Thomson weak coupling and Lotz fit.**
  - **via angular analysis vs energy of Rutherford, cross section at energy ε, to transfer energy $\Delta\varepsilon$ is:** $d\sigma = (\pi e^4/\varepsilon)(d\,\Delta\varepsilon/(\Delta\varepsilon)^2)$
  - **The cross section for transfer exceeding ionization energy E is:** $\sigma = (\pi e^4/\varepsilon)(1/E - 1/\varepsilon)$

- **Relativistic cross sections (J. Scofield, Phys. Rev. A 18, 963, 1978)**
  - **Born Diagram (neglect exchange - should be good for disparate electron energies)**
  - **relativistic plane waves for incident and scattered high energy electron, distorted waves & relativistic Hartree-Slater for ejected electron**

L-shell ionization



$$\sigma \quad \beta^{-2}\left[A\left[\ln\left(\beta^2/\left(1-\beta^2\right)\right)-\beta^2\right]+C\right]$$

Relativistic Electron IonizationCross Sections Scale Asymptotically like the Møller Cross Section (2)

• **Møller (electron-electron) Scattering including exchange (Ahkiezer & Berestetskii, Quantum Electrodynamics):**

$$d\sigma = \frac{r_0^2}{4v^4}\frac{[2(\frac{\varepsilon^2}{m^2})-1]^2}{\frac{\varepsilon^6}{m^6}}\{\frac{4}{\sin^4\vartheta}-\frac{3}{\sin^2\vartheta}+\frac{[(\frac{\varepsilon^2}{m^2})-1]^2}{[2(\frac{\varepsilon^2}{m^2})-1]^2}(1+\frac{4}{\sin^2\vartheta})\}d\Omega$$

• **v, ε, and θ are respectively the incident velocity, energy and scattering angle in the cm system.**

• **Energy Loss is conveniently expressed in terms of $\Delta=(\varepsilon_1-\varepsilon_2)(/\varepsilon_1$-m) = 1/2 (1-cos($\theta$))**

$$d\sigma = \frac{2\pi r_0^2}{v_1^2(x-1)}\frac{d\Delta}{\Delta^2(1-\Delta)^2}\{1-[3-(\frac{x-1}{x})^2]\Delta(1-\Delta)+(\frac{x-1}{x})\Delta^2(1-\Delta)^2\}$$

• **Note log behavior as well as small Δ behavior (recovering Rutherford for for energy loss (x=ε_1/m)**

The 'Ziman Formula' for Resistivity is the Workhorse for Liquid Metals and Warm Dense Plasmas – However it is an effective 'Boltzmann closure'

• **Ziman formula utility: typical structure factors S(q) for dense disordered 'metallic' media are peaked at the peak of the screened pseudopotential v_s(q) seen by conduction electrons**

$$\rho = \frac{6\pi^2}{h}\frac{1}{j_f^2}\frac{1}{N}\int_0^1 |v(q)|^2 S(q) 4(\frac{q}{2k_f})^3 d(\frac{q}{2k_f})$$

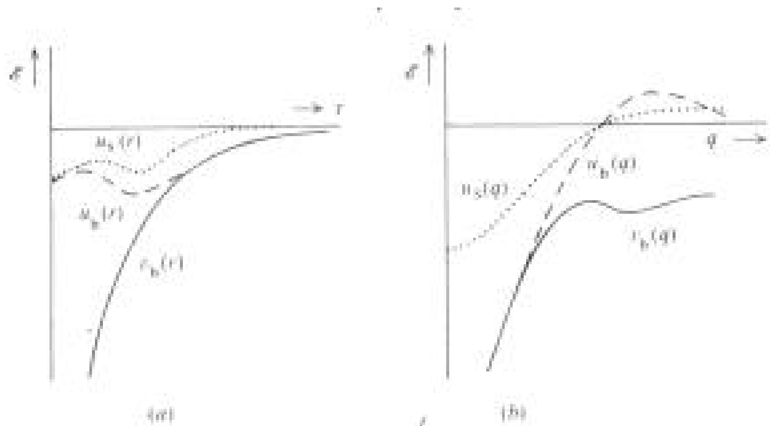


Fig. 10.3. Bare and screened pseudopotentials: (a) in real space; (b) in reciprocal space.

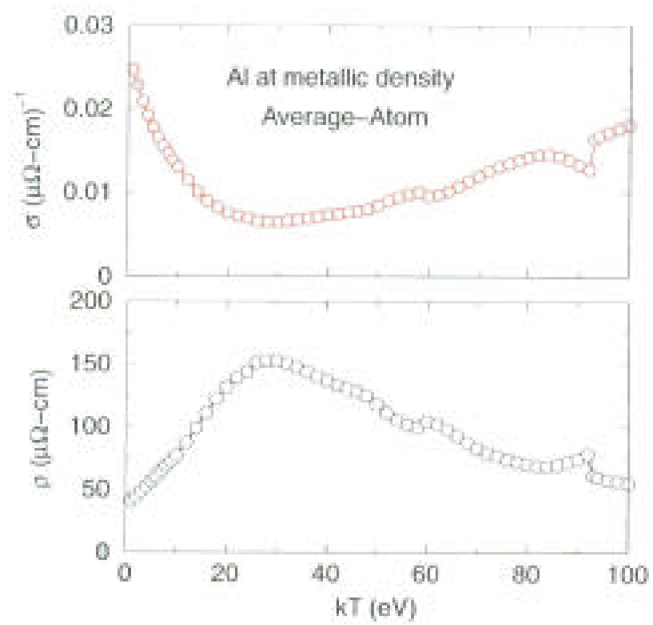


Figure 9: Conductivity σ and resistivity ρ of Al from the Ziman formula obtained using phase shifts from the average-atom code.

via G. Bertsch, C. Guet, and W. Johnson, finite temperature DFT calculation.

One Electron Treatment of the Many Impurity System without 'closures' enforcing 'average' relaxation times (after Doniach & Sondheimer, Smith & Rammer)

- **Kubo Formula for Linear Response Treatment of Conductivity (exact):**

$$\sigma = \frac{\pi e^2}{m\Omega} \sum_{\alpha} \sum_{\beta \neq \alpha} (p_x)_{\alpha\beta} (p_x)_{\beta\alpha} \delta(E_\alpha - E_\beta - \frac{h\omega}{2\pi}) \frac{f_\beta - f_\alpha}{\omega}$$

- **Calculations can have spurious divergences as ω goes to zero unless one is careful (note f sum rule). Molecular dynamics computations for wavefunctions in disordered 'warm dense matter' have shown interesting behaviors (Desjarlais).**

- **The Langer-Neal diagrams (*Phys. Rev. Lett.*, 1966) are the 'first set' of systematic corrections to Drude behavior to order e^2/h – coherent backscattering due to an arbitrary, random set of scatterers.**

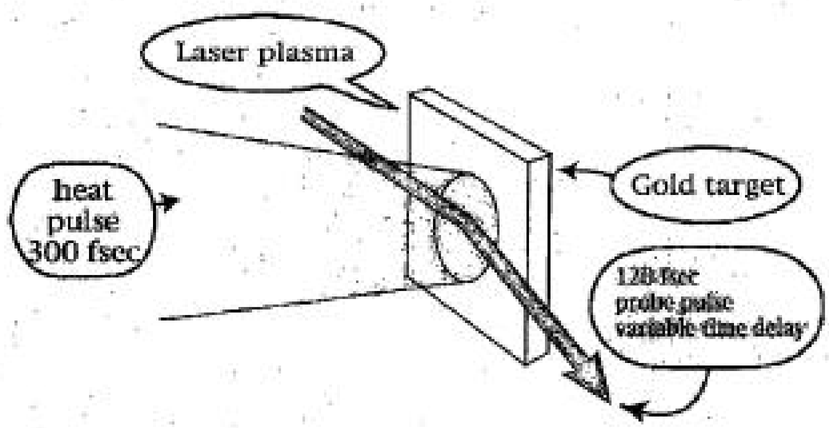
Short Pulse Laser and Pulsed Wire Array Experiments Producing 1- 5 eV expanded plasmas give surprising evidence for unusually low, finite ω, conductivities

- **Present Motivation:**
  - **Theory and experiment give evidence for conductivities below 'Ioffe-Regel' minimum 'metallic' conductivity for a variety of plasmas with**

$$\frac{1}{2}eV \le kT \le 5eV \qquad .0001 \le \frac{\rho}{\rho_{solid}} \le .1$$

  - **M. Desjarlais et. al., *Contrib. Plasma Phys*. 41 (2001), H. Yoneda et. al., *Phys. Rev. Lett.* 91, 075004 (2003).**
  - **Ioffe-Regel d.c. metallic conductivity minimum is**

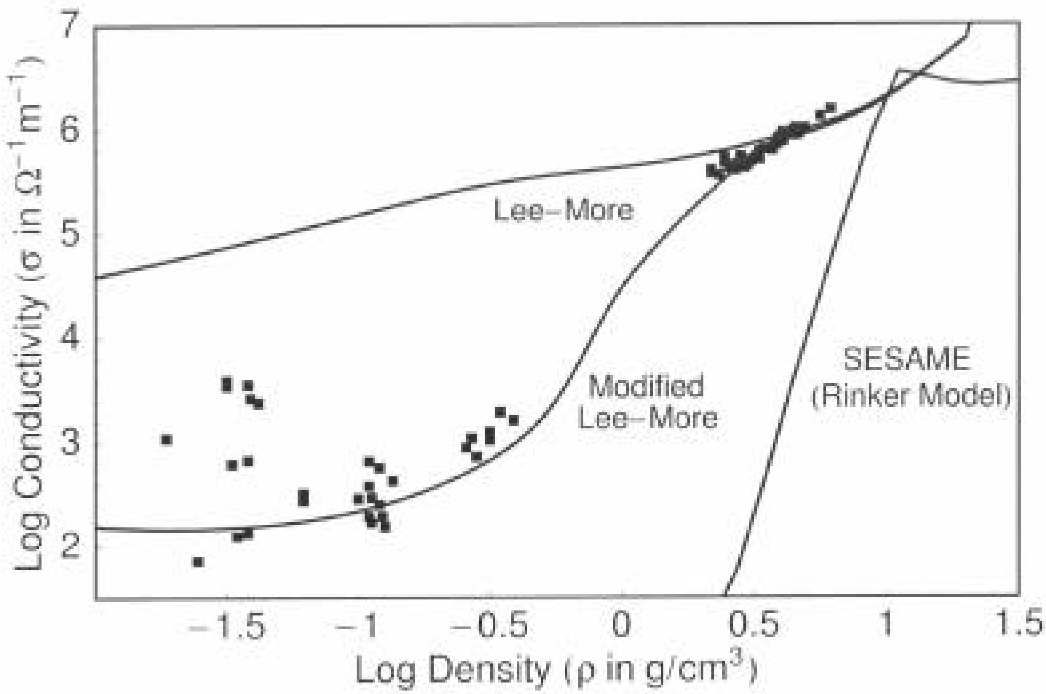
$$\sigma = \frac{2e^2 k_f^2 l}{3\pi h} \quad k_f l_{mfp} \approx 1 \Rightarrow \sigma = \frac{2e^2}{3\pi h l_{mfp}} \approx 10^2\,(ohm-cm)^{-1}$$



$$\varepsilon(\omega) = 1 + 4\pi n_a \alpha(\omega) + \frac{4\pi i \sigma(\omega)}{\omega}$$

Evidence that the conductivity component σ is anomalously small even after taking into account ionization balance!

Low Temperature and Density Anomalous Effects in the Equation of State and Electrical Conductivity*

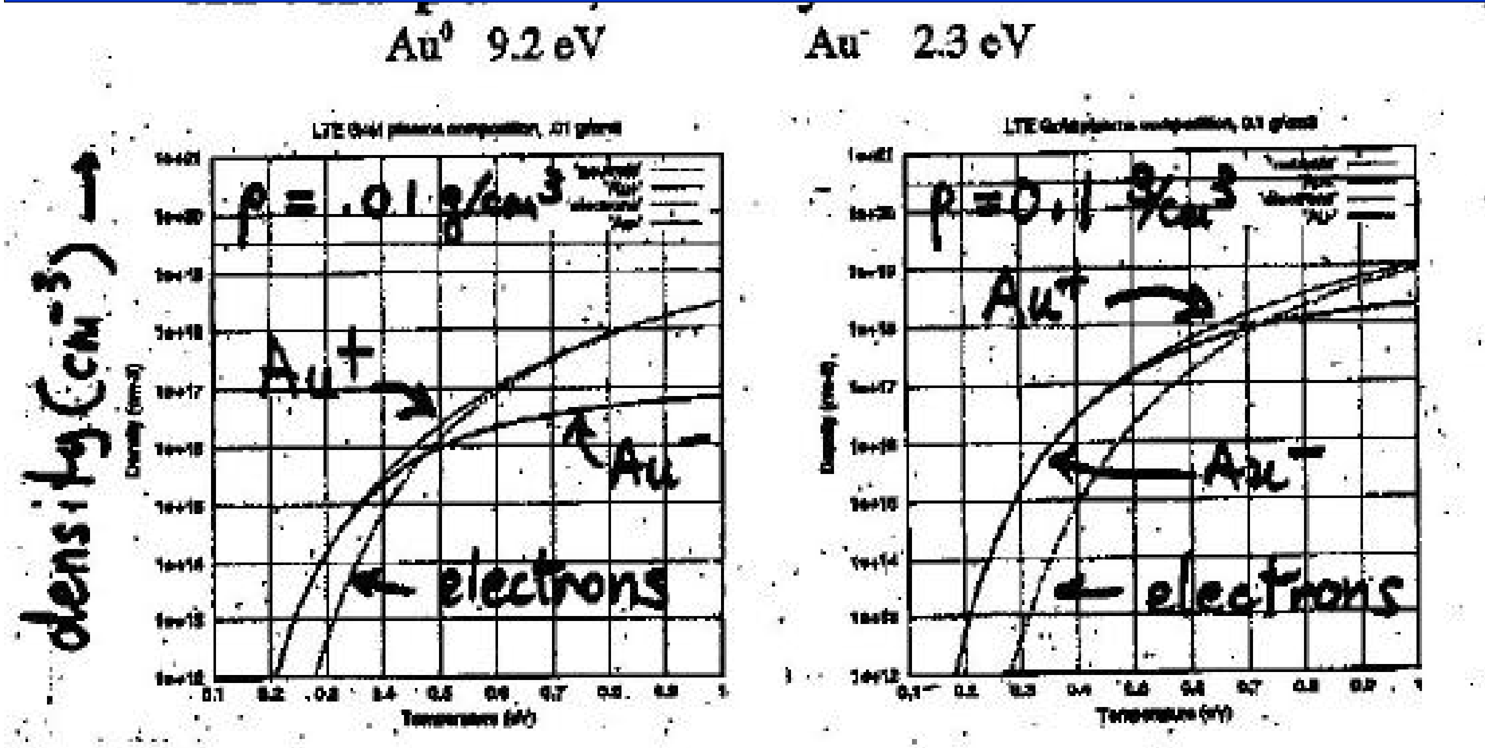


Lee-More model is a Drude type model with multiple mechanisms for n_e and τ in $\sigma = n_e e^2 \tau / m$ (including Mott minimum metallic conductivity).

Desjarlais's modified Lee-More model (blended Saha, pressure ionization, phenomenological e^- - neutral cross section - Contrib. Plasma Phys. 41, 2001, 267).

Need to add negative ions, as well as possible multi-center non average atom scattering.
***R. M. More, T. Kato, I. Murakami, M. Goto, H. Yoneda, G. Faussurier, M. Desjarlais, S. B. Libby to be published.**

Consequences of Au^- for ionization balance at low temperature and density - compensated semiconductor analog



Simplified Saha argument

$$\frac{n_+ n_e}{G_1(T)} = n_0 e^{-\frac{E_I}{kT}}$$

$$\frac{n_0 n_e}{G_2(T)} = n_- e^{-\frac{E_A}{kT}}$$

$$n_- + n_e = n_+$$

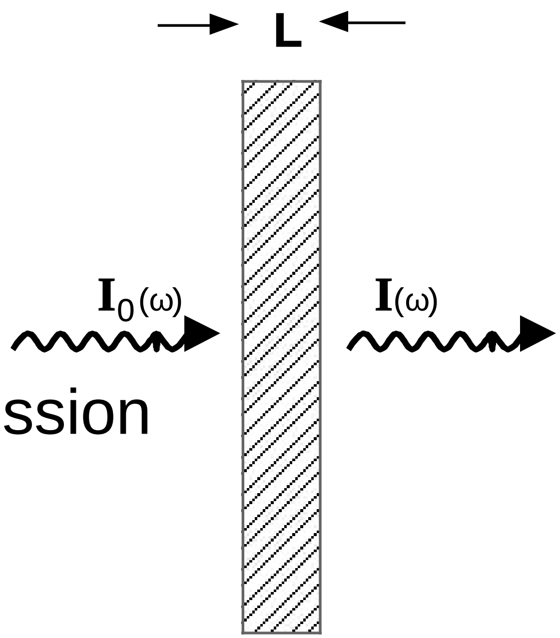
$$n_e \approx \left(\frac{8\pi mkT}{h^2}\right)^{\frac{3}{2}} e^{-\frac{E_I + E_A}{2kT}}$$

Au, Au+, Au-, and e- ρ vs. T as predicted by the Saha equation (R. M. More) for densities of .01 and .1 gr/cc revealing the relative importance of the negative ion Au- vs. free electrons. σ will depend on degree of 'compensation,' neutral scattering cross section, and non-average atom effects. Analogous results for Cu (affinity ~ 1.23 eV and I ~ 7.73 eV).

Radiation Transport Deals with Photon Emission and Absorption Following Fundamental Thermal Laws

- The transfer equation for radiation in 1-D can be written

$$\frac{dI_\nu}{ds} = \rho j_\nu - \left\{ \rho\kappa_\nu - \frac{\rho j_\nu}{\frac{2}{(hc)^2}(h\nu)^3} \right\} I_\nu$$



where

$$\rho j(h\nu) = n_j A_{ji} h\nu_{ij} \frac{\psi_\nu}{4\pi}$$ is the spontaneous emission

$$\rho\kappa(h\nu) = n_i B_{ij} h\nu_{ij} \frac{\phi_\nu}{4\pi}$$ the bare absorption

$$A_{ji} = \frac{2\left(h\nu_{ij}\right)^3}{(hc)^2} B_{ji}$$ and $g_i B_{ij} = g_j B_{ji}$.

B_{ji} is the stimulated emission coefficient

- ρ,κ depends on microscopic Quantum coefficients A&B,
  plasma thermal populations of lower and upper states $n_{i,j}$
  plasma influence on spectral profiles ψ_ν and φ_ν

Radiation Transport (continued)

- In general, populations depend on the plasma radiation field, and free electron distribution. Must close equations with microscopic rate equations depending on n_ν, T_e, n_e to get ρ & κ_ν. ("non - local thermal equilibrium" - NLTE - is hard!)

- *In the special case of LTE*, populations satisfy the Saha-Boltzmann relation characterized by a single temperature T_e (the electron temperature)

  - Then

$$\frac{n_j}{n_i} = \frac{g_j}{g_i} e^{-(E_j - E_i)/kT_e}$$

$$\frac{dI_\nu}{ds} = \rho\tilde{\kappa}_\nu \left(J_\nu - I_\nu\right) \qquad \tilde{\kappa}_\nu \equiv \kappa_\nu^{(LTE)}\left(1 - e^{-h\nu/kT_e}\right) \qquad j_\nu^{(LTE)} = \kappa_\nu^{(LTE)} \frac{2}{(hc)^2}(h\nu)^3 e^{-h\nu/kT_e}$$

$$J_\nu = \frac{2}{(hc)^2}\frac{(h\nu)^3}{e^{h\nu/kT} - 1}$$

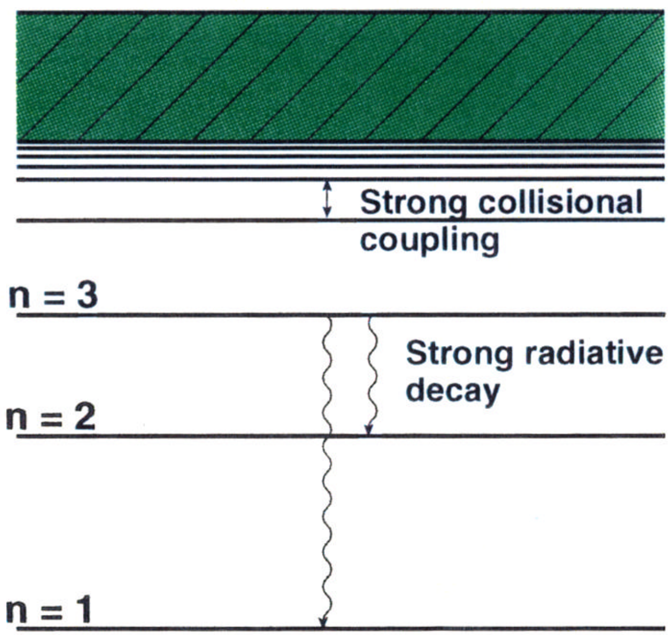
- *And in complete equilibrium the Radiation field is characterized by a Planckian distribution at the same temperature T_e=T_R*

Local Thermal Equilibrium (LTE) occurs when the ion populations are thermally characterized by the Maxwellian electron temperature T_e. Non-LTE occurs when this hypothesis fails.

- A simple model (Griem) for the electron density required to drive a given level n to LTE is

$$\sum_{m} C(n,m) + I(n) \geq 10 \sum_{m<n} A(n,m)$$

$$N_e(\mathrm{cm}^{-3}) \geq \frac{7 \times 10^{18}}{n^{8.5}} Z^7 \left(\frac{KT_e}{Z^2 E_H} \right)^{1/2}$$



Electron continuum and ion charge state Q + 1

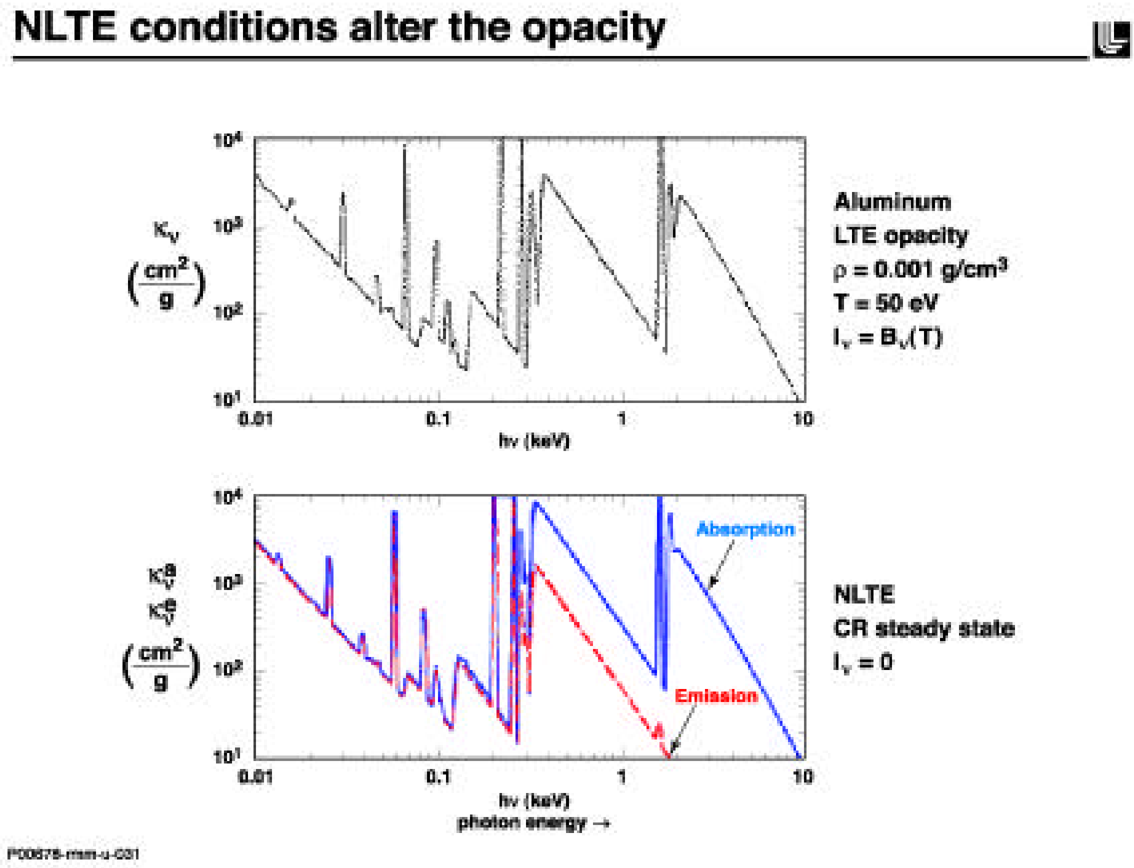
Rydberg states near LTE

"Isolated" levels often non-LTE unless sufficient collisions and/or radiation

Ground state of ion charge state Q

- Radiative effects play a key role in driving LTE in many situations
- Non-LTE effects are significant in laser-plasma experiments
- Our radiation transfer models often need to account for NLTE

NLTE Radiation Fields Effect the Emission and Absorption Opacities: Aluminum at .001 gr/cc and 50 eV



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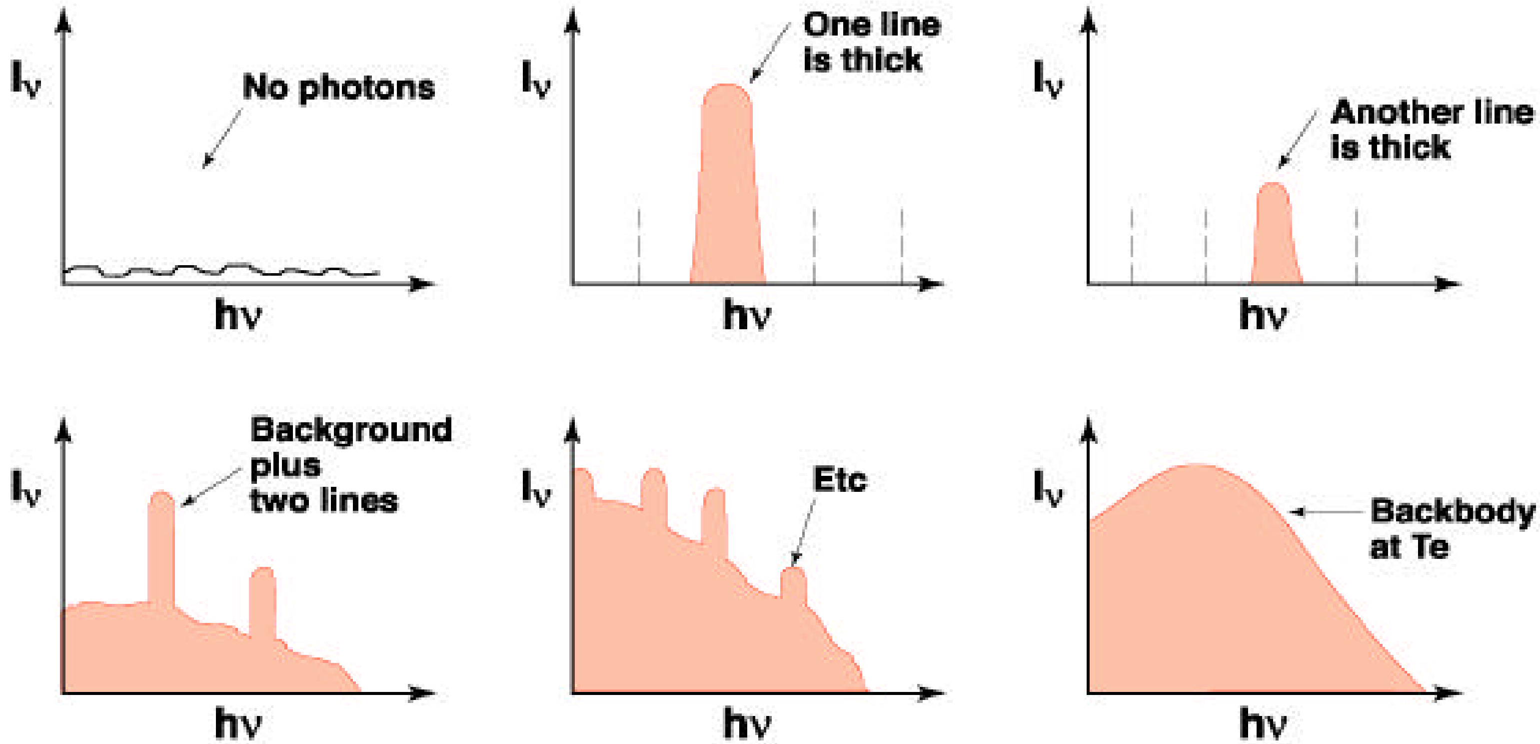
Non-LTE in a multi-dimensional space?



- Each photon frequency-group is another degree of freedom
- The state of the atom is determined by the set of variables ρ, Te, $\{I_\nu\}$

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The effect of radiation on non-LTE atomic kinetics in hot dense plasmas can be understood from the view point of non-equilibrium thermodynamics*

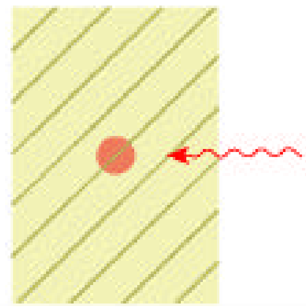
- Our Strategy: extract NLTE physics in simpler way near LTE limit avoiding computational explosion (complexity example: M shell iron - 10^3 configurations like $1s^2 2s^2 2p^6 3s 3p^2 3d 5d \rightarrow 10^6$-$10^7$ lines – as Z increases the number of lines grows fast!)
- Earlier ideas: for electron dominated plasmas, Pitaevski, Gurevich, and Beigman studied electron currents in principal quantum number space (L&L vol. 9); also Scovil and Schulz-Dubois analyzed the steady state maser as a Carnot engine, PRL 2, 1959. (also note analogous treatment of the Overhauser effect).
- We study the linear response of an LTE atom (ion) subject to a steady imposed radiation spectrum I_ν constituting effective temperature shifts δT_ν away from $B_\nu(T_e)$.
- The resulting Response Matrix in frequency group space $R_{\nu\nu'}$ naturally separates the problem of radiation – hydrodynamics from the underlying kinetics and lines.
- Because $R_{\nu\nu'}$ expresses entropy flow, it obeys Onsager constraints.
  – $R_{\nu\nu'}$ is symmetric and has a straightforward form in terms of the plasma rate coefficients. Consistency test for NLTE codes.
  – The principle of minimum entropy production is obeyed.
  – Computed examples in 3 NLTE models show a large range of linear response.
  – Inline $R_{\nu\nu'}$ tabulation scheme offers enormous NLTE rad-hydro acceleration.

- * Libby, Graziani, More, Kato, 13th conf. LIRPP, AIP 1997; More, Kato, Faussurier, Libby, JQSRT, 2001; DeCoster, JQSRT, 2001.

Many near-LTE plasmas can be analyzed using the linear-response method

Ion plus photon beam

- XRL interaction

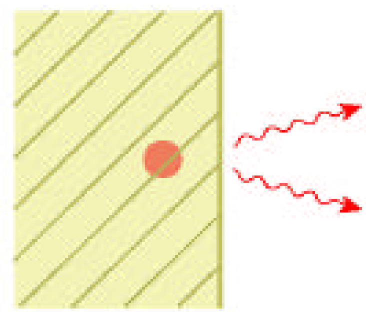


Ion
+
Electrons $T_e = T$
+
Photons $B_\nu(T) + \delta I_\nu$

Beam

Ion near boundary of medium

- Shock structure

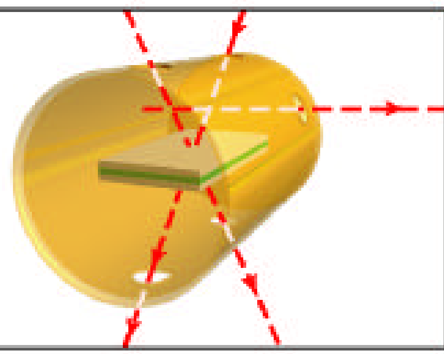


Ion
+
Electrons $T_e = T$
+
Photons $B_\nu(T) - \delta I_\nu$

Escaping photons

Ion in hohlraum

- Opacity experiment



Sample ion
+
Electrons $T_e = T$
+
Photons $B_\nu(T) + \delta I_\nu$

Small perturbation e.g., gold M-band

Near-LTE non-LTE is a precisely-defined class of states

ρ, T_e, $\{I_\nu\}$ — for 50 groups, a 52-dimensional space

Write $I_\nu = B_\nu\,(T_\nu)$

Near LTE, photon group temperature $T_\nu = T_e + \delta T_\nu$

Near LTE, expect

$$(\kappa_\nu^e - \kappa_\nu^a)\, B_\nu = \sum_{\nu'} R_{\nu,\nu'}\, \delta T_{\nu'} + O\,(\delta T^2)$$

$R_{\nu,\nu'}$ = linear response matrix for near-LTE non-LTE

Calculate $R_{\nu,\nu'}$ for ion in LTE with perturbation $\delta T_{\nu'}$

Photons at energy $h\nu'$ change the opacity at $h\nu$

The Linear Response Matrix R ν,ν' Controls All Possible Near Equilibrium Steady States - It Is Expressible in Terms of Microscopic Rates and Must Obey Onsager Relations

$R_{\nu,\nu'}$ is not the usual matrix of atomic rates

- $R_{\nu,\nu'}$ has a simple, fixed format
  - independent of ion stage
  - independent of coupling (jj, L.S, intermediate or C.I.)
  - same format for average-atom method
- $R_{\nu,\nu'}$ has a direct relation to the transport equation
  - "Read it and run" with no need to find or evolve eigenvectors
  - Does not require populations from previous time-step
- Describes quasi-steady plasma; omits transient effects

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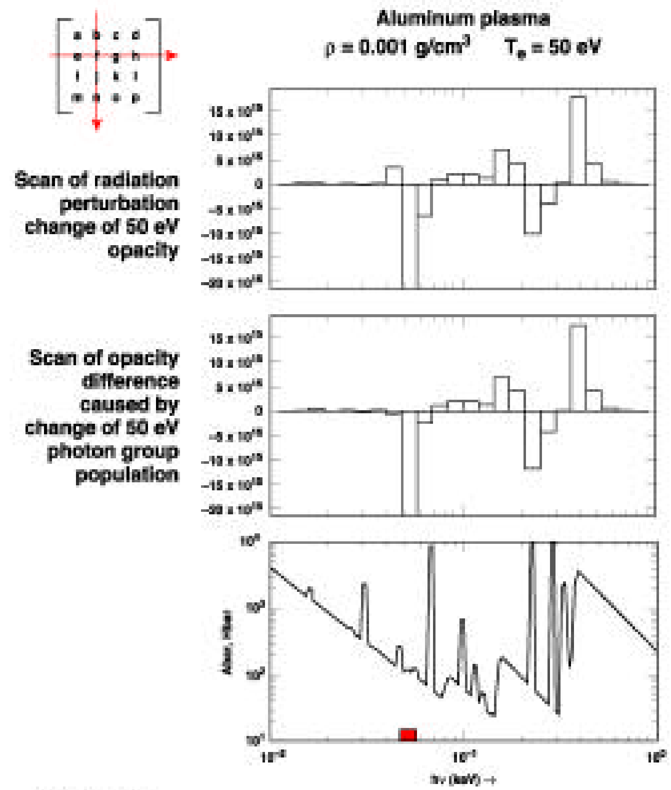
Screened hydrogenic model produces a symmetric response matrix $R_{\nu,\nu'}$



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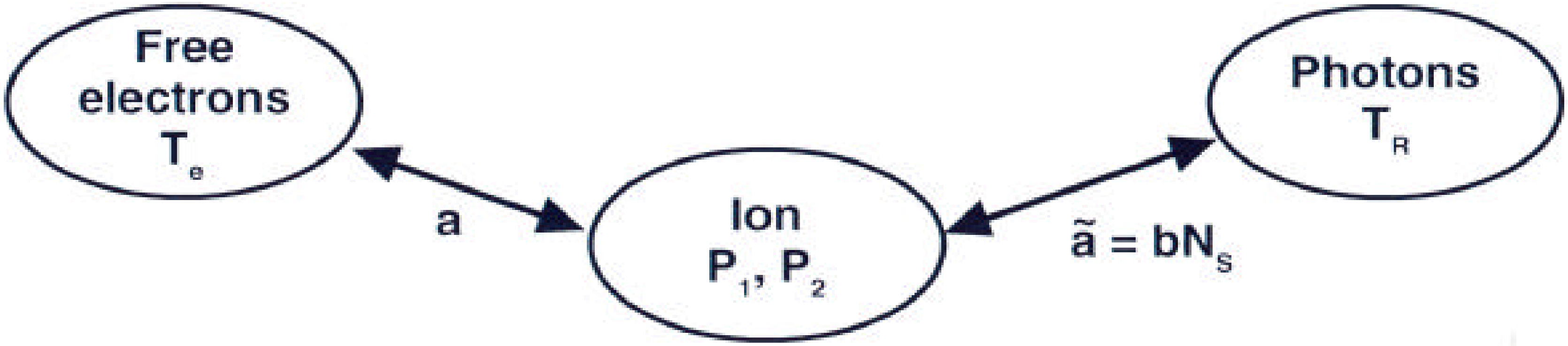
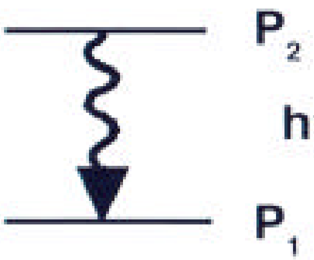
The non-equilibrium thermodynamics of steady state plasmas is exemplified by the coupling of a two level ion to distinct electron and photon heat baths





$$\frac{dP_1}{dt} = \underbrace{-aP_1 + ae^{\frac{E}{kT_e}} P_2}_{\text{Coupling to electrons;}} \underbrace{- bN_SP_1 + b(N_S + 1) P_2}_{\text{to photons}}$$

$P_1 + P_2 = 1$

Define $\tilde{a} = bN_S$; $N_S + 1 = e^{E/kT_R} N_S$ gives

$$\dot{P}_1 = (a\, e^{E/kT_e} + \tilde{a}\, e^{E/kT_R}) P_2 - (a + \tilde{a}) P_1$$

- The non-equilibrum state of the ion is precisely mirrored by the heat flow in the reservoirs when one is near LTE.

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The State of Minimum Entropy Production is Identical to the True Near Equilibrium Steady State

RATE OF ENTROPY PRODUCTION $\dot{S} = \dot{S}(P_1)$

$$S_{ion} = -k(P_1 \log P_1 + P_2 \log P_2)$$

$$\dot{S}_{ion} = -k\,\dot{P}_1 \log\left(\frac{P_1}{P_2}\right)$$

$$\text{Electrons } \dot{S}_e = \frac{E}{T_e}\left(\frac{dP_1}{dt}\right)_e$$

$$\text{Radiation } \dot{S}_R = \frac{E}{T_R}\left(\frac{dP_1}{dt}\right)_R$$

The total rate of entropy production $\dot{S}_{ion} + \dot{S}_e + \dot{S}_R$ is a function of the ion thermodynamic state $(\sim P_1^s)$.

True steady-state is determined by $\dot{P}_1 = 0$

$$P_1^s = \frac{a\,e^{E/kT_e} + \tilde{a}\,e^{E/kT_R}}{a(1 + e^{E/kT_e}) + \tilde{a}(1 + e^{E/kT_R})}$$

Near equilibrium we have $\begin{cases} T_e = \overline{T} + \delta T \\ T_R = \overline{T} - \delta T \end{cases}$; $P_1^o \equiv \dfrac{1}{1 + e^{-E/kT}}$

$$P_1^s = P_1^o - \frac{a - \tilde{a}}{a + \tilde{a}} P_1^o(1 - P_1^o)\frac{E}{k\overline{T}}\frac{\delta T}{\overline{T}} + 0(\delta T^2)$$

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STATE OF MINIMUM ENTROPY PRODUCTION:

$\dfrac{\partial \dot{S}}{\partial P_1} = 0$ is not (in general) equivalent to $\dfrac{dP_1}{dt} = 0$

However, if $\delta T \ll \overline{T}$ we obtain $\dfrac{\partial \dot{S}}{\partial P_1} = 0$ when

$$P_1 = P_1^o - \frac{a - \tilde{a}}{a + \tilde{a}} P_1^o(1 - P_1^o)\frac{E}{kT}\frac{\delta T}{T} + 0(\delta T^2)$$

The principle of minimum entropy production correctly characterizes the steady-state to first order in the departure from equilibrium ($\delta T/T$).

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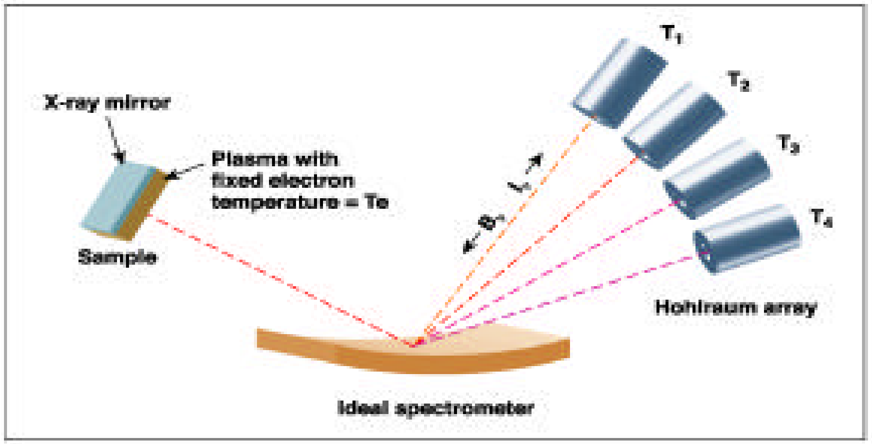
The General NLTE Steady State is Defined by Multiple Effective Temperature Boundary Conditions

Thermodynamics of steady near-LTE plasma is clarified by a thought-experiment — The NLTE Reaction Box



- Each hohlraum has a controlled temperature
- When all temperatures are equal, plasma is in LTE

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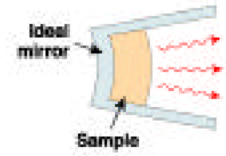
Thermodynamic analysis of the reaction box requires following the energy-flow



A = area
Ω = solid angle
d = thickness
($\rho\kappa_\nu d \ll 1$)

Energy flux from hohlraum = $A \cdot \Omega \cdot B_\nu(T_\nu)$

Return flow = input + $A \cdot \Omega \cdot 2\rho d\,(\kappa_\nu^a - \kappa_\nu^e)\,B_\nu$

Energy conservation:

$$\frac{dE_e}{dt} + \frac{2\rho d A\Omega}{4\pi} \sum_\nu \sum_{\nu'} R_{\nu\nu'}\,\delta T_{\nu'}\,\Delta\nu\,\Delta\nu' = 0$$

Entropy production in reservoirs:

$$\frac{dS}{dt} = \frac{1}{T_e}\frac{dE_e}{dt} + \sum_\nu \frac{1}{T_\nu}\frac{dE_\nu}{dt}$$

$$= \frac{2\rho d A\Omega}{4\pi} \sum_\nu \sum_{\nu'} \left(\frac{1}{T_\nu} - \frac{1}{T_e}\right) R_{\nu\nu'}\,\delta T_{\nu'}\,\Delta\nu\,\Delta\nu'$$

$$\approx \underbrace{-\left(\frac{2\rho d A\Omega}{4\pi}\right)}_{\text{Geometrical factor}} \frac{1}{T_e^2} \underbrace{\sum_\nu \sum_{\nu'} R_{\nu\nu'}\,\delta T_\nu\,\delta T_{\nu'}\,\Delta\nu\,\Delta\nu'}_{\text{Quadratic form}}$$

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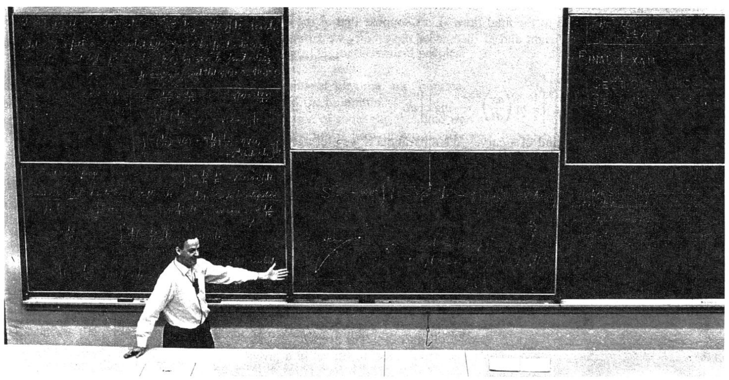
The Principle of Minimum Entropy Production has an Interesting History. Its Connection to other Variational Principles and Quantum Dynamics is Still Unknown!

Feynman Lectures
Volume II

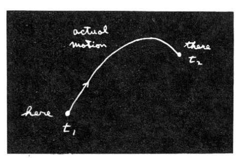
The Principle of Least Action



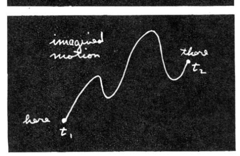
A special lecture—almost verbatim*

"When I was in high school, my physics teacher—whose name was Mr. Bader—called me down one day after physics class and said, 'You look bored; I want to tell you something interesting.' Then he told me something which I found absolutely fascinating, and have, since then, always found fascinating. Every time the subject comes up, I work on it. In fact, when I began to prepare this lecture I found myself making more analyses on the thing. Instead of worrying about the lecture, I got involved in a new problem. The subject is this—the principle of least action.

"Mr. Bader told me the following: Suppose you have a particle (in a gravitational field, for instance) which starts somewhere and moves to some other point by free motion—you throw it, and it goes up and comes down.



It goes from the original place to the final place in a certain amount of time. Now, you try a different motion. Suppose that to get from here to there, it went like this



but got there in just the same amount of time. Then he said this: If you calculate the kinetic energy at every moment on the path, take away the potential energy, and integrate it over the time during the whole path, you'll find that the number you'll get is *bigger* than that for the actual motion.

* Later chapters do not depend on the material of this special lecture—which is intended to be for "entertainment."

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Feynman Lectures
Volume II

A note added after the lecture

"I should like to add something that I didn't have time for in the lecture. (I always seem to prepare more than I have time to tell about.) As I mentioned earlier, I got interested in a problem while working on this lecture. I want to tell you what that problem is. Among the minimum principles that I could mention, I noticed that most of them sprang in one way or another from the least action principle of mechanics and electrodynamics. But there is also a class that does not. As an example, if currents are made to go through a piece of material obeying Ohm's law, the currents distribute themselves inside the piece so that the rate at which heat is generated is as little as possible. Also we can say (if things are kept isothermal) that the rate at which energy is generated is a minimum. Now, this principle also holds, according to classical theory, in determining even the distribution of velocities of the electrons inside a metal which is carrying a current. The distribution of velocities is not exactly the equilibrium distribution [Chapter 40, Vol. I; Eq. (40.6)] because they are drifting sideways The new distribution can be found from the principle that it is the distribution for a given current for which the entropy developed per second by collisions is as small as possible. The true description of the electrons' behavior ought to be by quantum mechanics, however. The question is: Does the same principle of minimum entropy generation also hold when the situation is described quantum-mechanically? I haven't found out yet.

"The question is interesting academically, of course. Such principles are fascinating, and it is always worth while to try to see how general they are. But also from a more practical point of view, I *want* to know. I, with some colleagues, have published a paper in which we calculated by quantum mechanics approximately the electrical resistance felt by an electron moving through an ionic crystal like NaCl. [Feynman, Hellworth, Iddings, and Platzman, "Mobility of Slow Electrons in a Polar Crystal," *Phys Rev.* **127**, 1004 (1962).] But if a minimum principle existed, we could use it to make the results much more accurate, just as the minimum principle for the capacity of a condenser permitted us to get such accuracy for that capacity even though we had only a rough knowledge of the electric field."

Still an open question!

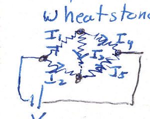
currents : analog of response

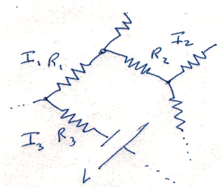
voltages : analog of 'force'

Onsager symmetry :

$$\frac{\partial I_i}{\partial V_j} = \frac{\partial I_j}{\partial V_i}$$

example : wheatstone bridge can be solved quickly!





$$\dot{S} = \sum_{\text{links}(i)} I_i V_i + \sum_{\substack{\text{nodes}\\(k,)}} \lambda_k \Big(\sum_{\text{in } k} I \Big)$$

power dissipation

constraint of current conservation

$$\frac{\delta \dot{S}}{\delta I_i} = 0 \Rightarrow \text{correct current pattern}$$

$$\frac{\delta \dot{S}}{\partial \lambda_k} = 0$$

uses

$$S = \sum_{i=1}^{5} I_i^2 R_i$$

$$+ \lambda_a (I - I_1 - I_2)$$

$$+ \lambda_b (I_1 - I_3 - I_4)$$

$$+ \lambda_c (I_2 - I_4 - I_5)$$

$$\frac{\partial S}{\partial I_1} = \frac{\partial S}{\partial I_5} = 0$$

eliminates need for Kirchoff voltage loops.

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